Meeting Enduring National Needs

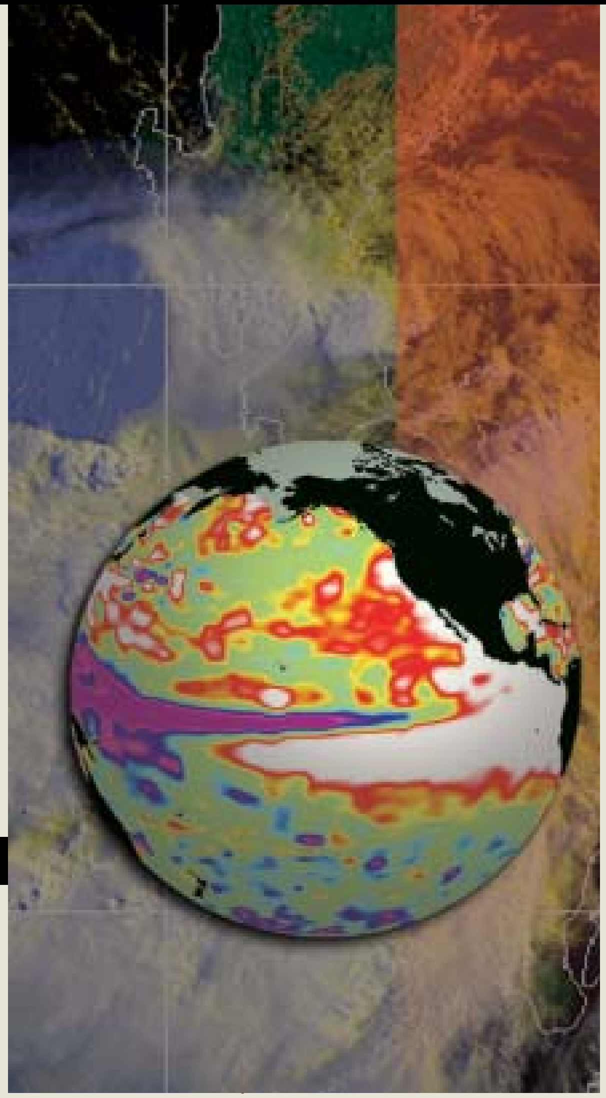
As part of its overarching national security mission, the Department of Energy pursues research and development in a variety of areas that are of enduring importance to the nation. In selected areas where the Laboratory can make valuable contributions, Livermore researchers support DOE mission priorities in energy and environment, bioscience, and fundamental science and applied technology. These activities make use of the Laboratory's multidisciplinary approach to problem solving, wide-ranging capabilities, specialized research facilities, and unique areas of expertise. Challenges are sought that reinforce the Laboratory's national security mission and have the potential for high-payoff results.

Long-term research is needed to help provide the nation with abundant, reliable energy together with a clean environment. Livermore's energy and environmental programs contribute to providing the scientific and technological basis for secure, sustainable, and clean energy resources for the U.S. and to reducing risks to the environment.

Bioscience research at Livermore enhances the nation's health and security. Leveraging the Laboratory's physical science, computing, and engineering capabilities, projects focus on molecular biology, genetics, computational biology, biotechnology, and health-care research. Research efforts are directed at understanding causes and mechanisms of ill health, developing biodefense capabilities, improving disease prevention, and lowering health-care costs.

In addition, initiatives are pursued in fundamental science and applied technology that reinforce strong research areas at the Laboratory. Many projects, sponsored by DOE's Office of Science and other customers, take advantage of the unique research capabilities and facilities at Livermore. Other work, supported by Laboratory Directed Research and Development funding, extends the Laboratory's capabilities in anticipation of new mission requirements.

Livermore's National Atmospheric Release Advisory Center (NARAC) provides real-time emergency predictions for hazardous substance releases.



The Climate Outlook: A Warming Trend

Computer simulations and data gathering by Livermore researchers are contributing to worldwide efforts to better understand the history of Earth's climate, changes due to human activities, and methods for mitigating the consequences.

One puzzle about climate change was addressed in a recent paper by Laboratory scientists and an international team: why satellite temperature measurements of the lower troposphere show little or no warming since such data collection began in 1979. Because these data, differing from other aspects of climate, have been used to support skepticism of global warming, the team decided to take a closer look. In their new study, sophisticated climate models separated the effects of recent major volcanic eruptions and El Niños from other causes of climate change. Remarkably, the results showed that large volcanic eruptions—El Chichón in 1982 and Mount Pinatubo in 1991—had a cooling effect on the lower troposphere that masked the overall warming trend shown in surface temperature data and brought about by human activities.

The natural variability of climate was the subject of a data-gathering trip in 2002 to the Gulf of Alaska by a team, including a Livermore scientist, sponsored by the National Oceanographic and Atmospheric Administration's Ocean Explorer Program. More than one ton of samples of seawater, coral, and sediment from the ocean floor was gathered by the Alvin submersible as deep as 3,800 meters. At Livermore's Center for Accelerator Mass Spectrometry, the isotopic profiles of the corals are being studied to better understand climate–ecosystem variability in the Gulf of Alaska over the last few hundred years. The sediment samples will tell a longer story—up to 250,000 years—at lower resolution.

Many other studies and collaborative research of climate change are ongoing, including completion of global climate simulations at the highest resolution yet performed (50 kilometers). In addition, computer studies are providing insights into the utility of injecting carbon dioxide deep in the ocean to sequester the greenhouse gas for centuries so that it does not contribute to global warming.

E. O. Lawrence Award for Ben Santer

In 2002, Ben Santer, a physicist in the Laboratory's Program for Climate Model Diagnosis and Intercomparison, received an E. O. Lawrence Award. The award cited "his seminal and continuing contributions to our understanding of the effects of human activities and natural phenomena on the Earth's climate system." Among his many contributions to the field, Santer was lead author of the critically important Chapter 8 of the *1995 Second Assessment Report of the Intergovernmental Panel on Climate Change*. The report concluded that "the balance of evidence suggests a discernable human influence on global climate"—a conclusion that has grown stronger as a result of continuing research on climate change. In 1998, Santer received a MacArthur Foundation "genius award."

Fuel Cells for Portable Electronics and Efficient, Clean Power

Livermore's Center for Microtechnology Engineering has developed and demonstrated a prototype miniature fuel cell that may provide portable electric power for consumer electronics as well as for sensors for military and security applications. Using easy-to-store liquid fuels such as methanol, the thin-film fuel cell power module is lighter weight than rechargeable batteries and provides more than three times the operating time.

The power module incorporates a thin-film fuel cell and microfluidic fuel-processing components in a common package (photo at right). The patented design and method for making the fuel cells combine microcircuit processes, microfluidic components, and microelectrical-mechanical systems (MEMS) technology.

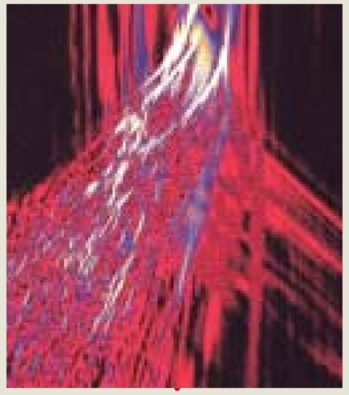
Livermore researchers are also improving the design of solid-oxide fuel cells, with the goal of making the technology an effective option for clean and efficient power generation for the 21st century. Solid-oxide fuel cells are particularly attractive because of their high efficiency. By applying materials science expertise, scientists are developing a very-high-power-density prototype that operates at a temperature low enough so that more affordable materials and manufacturing technologies can be used. A prototype modular fuel cell, consisting of a stack of three single cells, has been built and tested at the Laboratory. It achieved a power density of 1.05 watts per square centimeter at 800 degrees Celsius, a result for a stack of cells that is at least 50 percent higher than previously reported.

Materials Testing and Modeling for the Yucca Mountain Program

In February 2002, President Bush endorsed the DOE's recommendation to store high-level nuclear waste in an underground repository at Yucca Mountain, Nevada, and Congress subsequently provided its support for DOE's decision. For the Yucca Mountain Program, Livermore has played a major role in materials testing and performance modeling for the storage canister and system of engineered barriers surrounded by natural barriers to contain the radioactive waste. Laboratory researchers are now working to support major project milestones toward license application. In these efforts, significant emphasis has been placed on achieving high quality assurance.

At the Laboratory's Long-Term Corrosion Test Facility, researchers are conducting materials performance tests to confirm that the waste packages will maintain their integrity for thousands of years. Some 20,000 test specimens are currently being exposed or have been tested to expected conditions in vessels that simulate the bounding chemical and thermal conditions in the repository. In addition, new codes are being used to simulate the geologic evolution of the repository, predict the temperature evolution surrounding the buried waste, and explore the possible means by which water could enter the repository tunnels over geologic time periods.

Fusion Energy Science Progress on Many Fronts



In 2002, Laboratory researchers advanced fusion energy science through computational and experimental work on both inertial confinement fusion and magnetic fusion performed primarily for DOE's Office of Science. In the area of magnetic fusion energy, Livermore collaborates in experiments using the DIII-D Tokamak at General Atomics in San Diego and provides leadership in the development and use of computational models, such as UEDGE and BOUT, to study turbulence and other physical phenomena at the edge of the plasma (image at left). Recent BOUT calculations compare favorably with experimental data from the DIII-D and other tokamaks. Capabilities at Livermore can greatly contribute to U.S. participation in the International Thermonuclear Experimental Reactor (ITER) project.

In addition, Livermore is the site of the Sustained Spheromak Physics Experiment (SSPX), an alternative to the tokamak concept that may lead to lower-cost fusion reactors because of the spheromak's compact size and reduced complexity. In 2002, experimenters measured plasma temperatures greater than 300 electronvolts. The result is two times higher than temperatures attained at the beginning of the year and higher than previously reported measurements for any driven spheromak plasma.

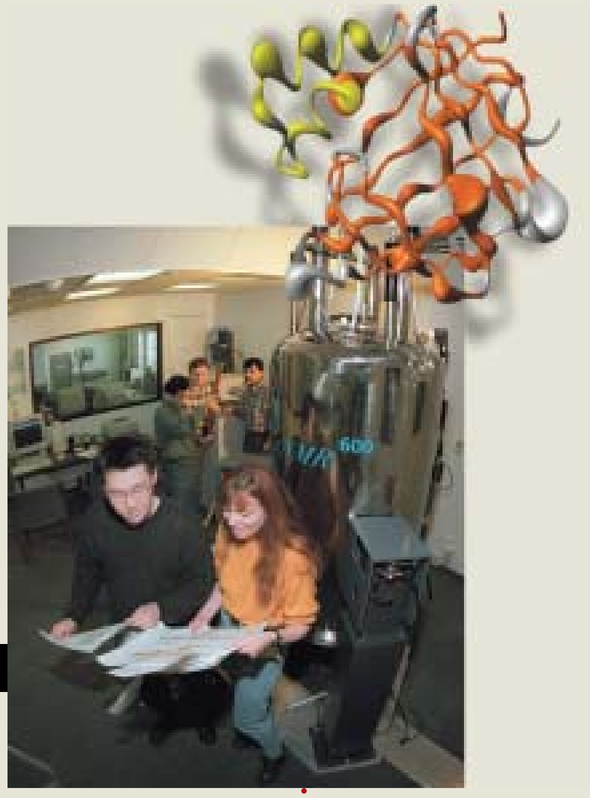
With the National Ignition Facility under construction, Livermore also provides international leadership in research in inertial confinement fusion. In collaboration with Lawrence Berkeley National Laboratory and others, Livermore researchers are investigating the concept of using a heavy-ion accelerator as the driver in an inertial fusion power plant. The effort reached a major milestone in 2002 with the dedication of Livermore's STS-500 (photo at left) and first experiments using the 500-kilovolt ion-source test stand. The STS-500 will be used for experiments addressing physics issues associated with the formation and behavior of heavy-ion beams.

Livermore's New Unclassified Supercomputer in the Top Five

To meet the growing needs of all of Livermore's programs for high-performance computing, the Laboratory acquired a new unclassified supercomputer, the Multiprogrammatic Capability Resource (MCR) machine, which complements the computing resources made available to the Stockpile Stewardship Program through NNSA's Advanced Simulation and Computing (ASCI) program. The MCR supercomputer was delivered during summer 2002 and became fully operational by October 31, when it was named the world's fifth fastest computer by Top 500, a supercomputing Website. The machine dramatically increases Livermore's unclassified computing capability. It is being used to support important projects in biology, materials science, lasers, and atmospheric science. Classified computing is accomplished on the Laboratory's more powerful ASCI White machine.

Using Linux cluster architecture, MCR provides 2,304 processors capable of performing 11.2 trillion calculations per second. Built by Linux NetworX and Quadrics, it is the first Linux-based supercomputer to be ranked in the top 10. At a cost of less than $14 million, MCR is a factor of 10 less expensive than the other top-ranked supercomputers. In the "operations per dollar" category, MCR ranks number one.

Experiments and Simulations to Predict Protein Structure



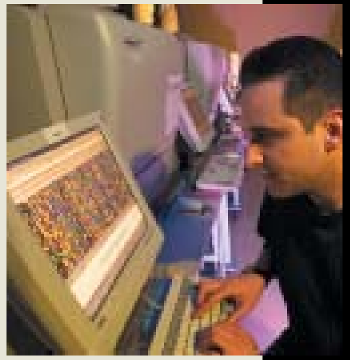
Researchers at the Laboratory are engaged in experimental and computational efforts to determine the structure of proteins. The three-dimensional structure of a protein offers clues as to its role in the body. This information can also be used to develop new diagnostic tools or therapies. Currently, structures are known for only a small percentage of the proteins that have been sequenced. Sequence data continues to accumulate at a rate that outpaces experimental data, which is gathered using x-ray crystallography and nuclear magnetic resonance spectroscopy. Methods of structure modeling and computational prediction are helping to close the information gap, for example, by extending the structural information to proteins within the same sequence family. Simulation tools are benefiting from dramatic increases in computer performance; however, fully predictive modeling tools have not yet been developed.

The Protein Structure Prediction Center at Livermore is coordinating two efforts for the sequencing community to help speed up the work. A critiquing process developed at the Laboratory called CASP (critical assessment of techniques for protein structure prediction) tests various prediction methods in advance of the experimental structures being released to the public. In addition, a related initiative, dubbed the "Ten Most Wanted," focuses modeling efforts on a small set of biologically important proteins whose structures are otherwise not expected to be determined experimentally in the near future.

Strides in Understanding the Function of Genes

In July 2002, an international consortium led by the Joint Genome Institute (JGI) reported work in *Science* magazine on draft sequencing, assembly, and analysis of the genome of the Japanese pufferfish, *Fugu rubripes*. Pufferfish have the smallest known genome among vertebrates, the group of animals with backbones that includes humans. By comparing the human and pufferfish genomes, researchers were able to predict the existence of nearly 1,000 previously unidentified human genes. Earlier, the JGI, which is operated by the three University of California–managed national laboratories, sequenced mouse DNA related to human chromosome 19 to compare the genes of the two species. Determining the existence and location of genes helps scientists to begin characterizing how genes are regulated and function in the human body.

Especially important now is discovering novel sequences that play a role in determining where and when genes are turned on or off, because understanding normal gene function is the first step in predicting disease mechanisms. Toward this longtime goal, Livermore scientists are using comparative sequence analysis, simultaneously examining DNA sequences from multiple organisms, to identify elements that are conserved over evolutionary time periods. Such conservation often signals that an individual sequence is important, perhaps because it is a gene or an element that regulates the expression of a gene. This approach has recently been used to identify potentially new regulatory pathways for gene expression and to suggest mechanisms by which genes can take on new functions.



A New Tool to Detect Genetic Variation and Cancers

The immense international research effort to map, sequence, and understand the human genome has led to the development of new tools for biological research. One new tool developed by a Livermore team can detect single damaged or missing DNA bases within individual cells, the smallest unit of genetic information, and thereby can significantly improve current methods of detecting cancer and other diseases. In 2002, the new technique, called in situ rolling circle amplification (IRCA), garnered one of the 100 awards presented annually by *R&D Magazine* to honor the most technically innovative products of the year.

IRCA is a fast and inexpensive method to precisely locate a damaged or abnormal gene that indicates the presence of or a tendency toward a particular disease, making IRCA ideal for analyzing tissue biopsies. In addition, IRCA provides answers in a couple hours, compared to a wait of several days required with tests using traditional methods.

Award-Winning Solid-State Laser Technologies

In 2002, two solid-state laser technologies developed at Livermore earned R&D 100 Awards. One winner was the solid-state heat-capacity laser (SSHCL), developed with industrial partners and sponsored by the U.S. Army Space and Missile Command. The refrigerator-size SSHCL can produce up to 13,000 watts in a single, high-quality beam with output pulse energies of more than 600 joules, making it the most powerful solid-state laser in the world. A 6-second shot of laser light from the system can bore a 1-centimeter-diameter hole in a 2-centimeter-thick plate of steel. In the past, this sort of fire power was available only from large gas or chemical laser systems. A larger laser that will produce 100,000 watts in a single beam is being developed. It will open up a range of applications for industrial materials processing and military defense.

The power of the SSHCL would be considerably higher if the flashlamp-pumped lasers in the system were replaced with a new diode-pumped solid-state laser technology, which also won an R&D 100 Award in 2002. This Livermore-developed technology, called SiMM (silicon monolithic microchannel), relies on photolithography and high-production etching techniques to produce thousands of miniscule, 30-micrometer-wide channels in silicon substrates. Water flowing through these microchannels cools the laser diode bars that are attached to the silicon, allowing the diodes to perform at higher average power than previously possible. To date, Livermore has fabricated arrays that measure just 10 by 18 centimeters and produce up to 45 kilowatts of power.

High-Data-Rate Laser Communication Demonstrated

Laser communication technology took a major step forward in 2002 with successful demonstration of an open-air link between the Laboratory and Mount Diablo, 28 kilometers apart. The Secure Air–Optic Transport and Routing Network, or SATRN, is a Laboratory Directed Research and Development project to meet the need for timely, secure, and economically practical data transmissions that exceed the capacity of radiofrequency and microwave systems. The challenge is to demonstrate an extended-range laser communication link with a high availability rate and a low bit-error rate. In 2002, the SATRN team collected data at a rate of 10 gigabits per second (contrasted with 270 megabits using radiofrequency links) without creating an information bottleneck by using four 2.5-gigabit-per-second channels operating at slightly different wavelengths. Livermore-developed adaptive optics systems, their use already proven in astronomical observatories, are key to the enhanced laser communication capability. The SATRN team is extending the concept's viability through efforts to increase the data rate to 40 to 100 gigabits per second and improve operability in varying weather conditions.

Adaptive Optics for Exploring the Solar System and Improving Vision

The Laboratory is at the forefront of developing adaptive-optics systems, which sense and correct aberrations, for a variety of applications. Livermore researchers are key partners in the Center for Adaptive Optics, a National Science Foundation Science and Technology Center, located at the University of California at Santa Cruz. In June 2002, Laboratory staff who are founding members of the center participated in the dedication of the center's new building.

In astronomy, Livermore-developed adaptive optics at the Keck Observatory in Hawaii (left) are enabling astronomers to minimize the blurring effects of Earth's atmosphere, producing images with unprecedented detail and resolution. They are now able to measure the shapes and sizes of asteroids, monitor weather patterns on Titan and Neptune, and image the faint rings of Neptune and Uranus (image below). A 20-watt dye laser built at the Laboratory has been installed on the Keck telescope to produce an artificial guide star, which allows adaptive-optic corrections to be made when viewing an object anywhere in the sky.

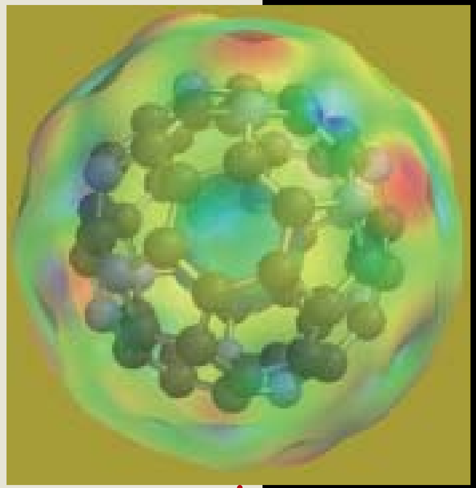
Researchers are also developing adaptive optics to study the human eye and to help in the early detection of eye disease. This new generation of prototype clinical adaptive-optics system is based on compact MEMS (microelectrical-mechanical systems) technology being developed at Livermore in partnership with industry and academia. These new systems will be used to study the limits of human visual acuity, which will guide improvements in contact lenses and laser refractive surgery.

Osmium Is Stiffer than Diamonds

The stiffest materials also tend to be the hardest ones. But in the case of diamonds and osmium, the former is still the harder even though the latter is stiffer. This surprising information was discovered by a Laboratory physicist who decided to study osmium because its stiffness had never been accurately measured. He crushed the osmium under 60 gigapascals of pressure in a diamond-anvil device and measured the resulting x-ray diffraction pattern to determine the spacing between osmium atoms. Osmium was found to have a bulk modulus—a measure of stiffness, or resistance to compression—of 462 gigapascals compared with 443 gigapascals for diamond.

A New Spin on Buckyballs

A high school student and a college student working at the Laboratory over the summer teamed up with a Livermore chemist to uncover an exciting new variant of a buckyball that includes nitrogen. The buckyball, or buckminsterfullerene, is a harder-than-diamond material consisting of 60 carbon atoms forming a molecule with a hollow core and perfect "soccer ball" symmetry. In analyzing the work of chemists who synthesized a fullerene material consisting of 48 carbon and 12 nitrogen atoms, the Livermore team found in its calculations a novel, more complex structure of these atoms that would be even more stable than the synthesized molecule.



With the team's results published, buckyballs bounced back into science news. Scientists have been interested in synthesizing fullerenes using other elements such as nitrogen to fine-tune properties that do not exist in C_{60} and reduce the cost of producing nanostructured materials. The new $C_{48}N_{12}$ material is highly elastic, resilient, and hard, ideal for such applications as orthopedic implants. It also provides a basis for synthesizing other nitrogen-substituted fullerenes with novel structural, electronic, and conducting properties.